Dimethylglyoxime
95-45-4 | DTXSID2044393

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 4.91e-01

Global applicability domain: Inside

Local applicability domain index: 4.94e-01

Confidence level: 6.39e-01

Nearest Neighbors from the Training Set

Image not found
N-Nitrosopyrrolidine
Measured: -0.190
Predicted: 8.73e-02

Image not found
N-Nitrosopiperidine
Measured: 0.36
Predicted: 4.99e-01

Image not found
Nitroso-1,2,3,6-
tetrahydropyridine
Measured: 1.18
Predicted: 8.43e-01

Image not found
Furazan, dimethyl-
Measured: 0.71
Predicted: 4.56e-01

Image not found
N-Nitrosodiethylamine
Measured: 0.48
Predicted: 4.93e-01